PROGRAM facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Power Systems Advanced Research

09/2004

COMPUTATIONAL ENERGY SCIENCES PROGRAM

Description

As market, policy, and regulatory forces reshape the energy industry, both domestically and globally, investments in advanced fossil energy technologies can return public and economic benefits many times over. One means of achieving these benefits is through the development of advanced coal technologies that use domestic fossil resources more efficiently and in an environmentally responsible manner. The Computational Energy Sciences (CES) Program is vital to achieving the Department of Energy's mission by providing technical information and a scientific, technical, and educational foundation on which improvements in the utilization of fossil energy can be realized. This allows the industries of the United States to be more economically competitive in a global economy.

The CES Program for fossil energy systems will provide an important basis for the Advanced Research (AR) and the Fossil Energy (FE) program to, in a short time, incorporate into its ongoing programs the enabling capabilities of scientific understanding facilitated by high speed computing. This will ultimately provide substantial saving in program costs by reducing the number of experimental studies and will, at the same time, compress development times for new technologies.

Goals

The overall goal of the simulation and modeling component of the CES Program is to provide simulation and computational resources to the FE programs which will speed the development and reduce the costs of new technologies. Specific goals for the CES include:

- Develop science-based models for the physical phenomena occurring in fossil fuel conversion processes;
- Develop simulation capabilities that calculate fluid flow, chemical reaction, heat generation, heat and mass transfer, and electrochemistry for modeling multi-dimensional transients in fuel cells, heat engines, combustors, gasifiers, chemical reactors, and other important equipment items in advanced power generation systems;
- Develop integrated simulation capabilities that couple science-based equipment models with overall system analysis models;
- Acquire access to multiple high end computing platforms for use in fossil energy simulations;
- Develop software for the simulation of fossil energy systems which can utilize teraflop computing resources;

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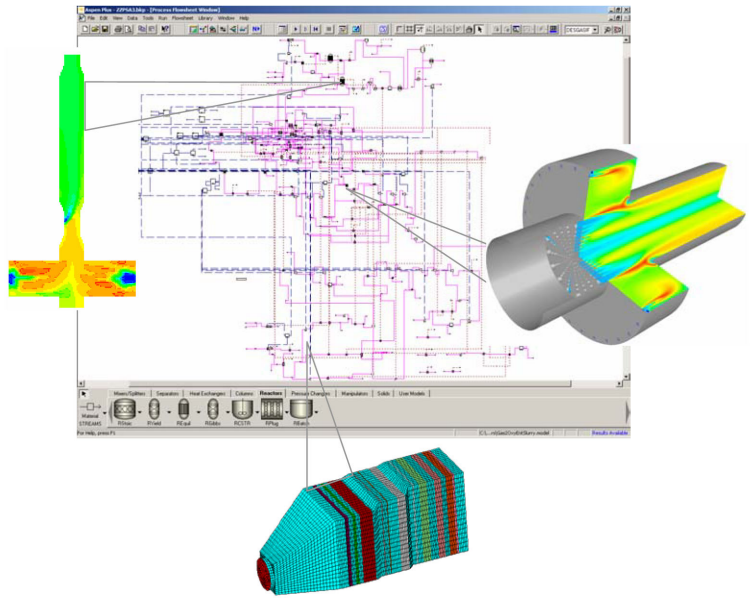
- Develop data reduction, data extraction and data mining techniques to utilize the extensive information made available from simulation studies of advanced power generation systems;
- Develop advanced data visualization capabilities for fossil energy simulation and experimental data display and analysis;
- Develop a "colaboratory" with NETL, multiple national laboratories, and universities which will provide extensive simulation and modeling expertise for advanced power generation systems. The expertise can be quickly mobilized in a cooperative dynamic working environment;
- Train student engineers and scientists to develop and analyze optimal control systems for future fossil energy plants; and
- Promote the use of simulation as a principle design, construction and operating tool for fossil energy equipment developers, suppliers and energy plant owners.

Program Areas

(1) Device-Scale, Systems, and Multiphase Flow Modeling and Visualization—Develop simulations that couple fluid flow, heat and mass transfer, chemical reaction, heat generation, and electrochemistry for modeling fuel cells, heat engines, gasifiers, and other critical processes in advanced power plants.

(2) Supercomputing Scientific Consortium (SC^2)—Continue to provide support to NETL in computational energy science and simulation.



An advanced power plant simulation (integrated gasification combined cycle with CO_2 capture) coupling process simulation and computational fluid dynamics models of a gasifier, turbine combustor and heat recovery steam generator. This work is a joint effort by the National Energy Technology Laboratory, Fluent, EG&G, and Alstom Power.

Benefits

Integrated Device-Scale and Process Simulation

- Accounts for impact of fluid dynamics, heat and mass transfer, and chemical reactions on overall process performance and efficiency
- Considers device-scale models in the context of process simulations, with recycle loops, heat integration, and other process units
- Enables analysis and optimization of overall process with respect to device-scale model parameters
- Represents necessary step in the development of "virtual" models
- Reduces the time, cost, and technical risk of developing advanced power generation systems